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AUTHOR(S): Robert B. Walker

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los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

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AN L^2 APPROACH TO R-MATRIX PROPAGATION: FOLLOWUP REPORT

by

Robert B. Walker
Theoretical Division
Los Alamos Scientific Laboratory
Los Alamos, New Mexico 87545

ABSTRACT

A hybridized R-matrix propagation program was used to solve the four test problems presented by the NRCC workshop on close coupling methods. The hybrid method used both the L^2 approach reported earlier and the analytic (constant reference potential) method. This report presents observations on the utility of the hybrid approach.

I. INTRODUCTION

In order to solve the test problems presented by the NRCC close coupling workshop, a program was written which combined the L^2 R-matrix propagation method discussed earlier[1] with the "standard" (analytic) R-matrix propagation technique.[2] The L^2 method is used to initiate the integration in the hard wall region of the potential, because it is independent of the potential variation within an R-matrix sector. We then switch over to the analytic method as the potential flattens out to take advantage of the cheaper (first energy) solution of the coupled equations in this region.

II. DISCUSSION

Because of the hybrid nature of the method used, it is significant to report in Table I the integration regions covered by each method for each of the test problems. The L^2 method is used in the interval from R_1 to R_2, and the analytic method is used from R_2 to R_3. The number of L^2 boxes is N_{BOX}, and the sector width of each box is $(R_2-R_1)/NBOX$. The analytic R-matrix propagation method is used from R_2 to R_3, and in this interval, N_{PROP} steps were taken. The L^2 method requires diagonalizing a matrix of size $N_D \times N_D$ once in each box at the first energy whereas the analytic method requires diagonalizing only a matrix of size $N_{CHAN} \times N_{CHAN}$ once each step at the first energy. Because these diagonalizations are not done after the first energy, the second energy timing is substantially faster than the first. The extremely large matrix which must be diagonalized in the L^2 region effectively limited the total number of coupled equations which could be handled by this program. For this reason, only the first three basis sets for each test problem were solved. The number of translational functions associated with each coupled channel can be figured out from Table I as $N_{TF} = N_D/N_{CHAN}$.

A more detailed analysis of the timing for the hybrid method is presented in Table II for the third basis set of test problems 1, 2a (J=5), 2b (J=25), and 4. These tables show clearly that the principal effort for this method is expended near the beginning of the integration region. For this reason, it is essential to remember to optimize the starting point (R_1 in Table I) of the integration when using this method. In all the problems used here, R_1 could have been made larger than it was, with a significant decrease in execution times. For example, in the 18-channel basis of test problem 1, fully one-third of the total execution time would have been eliminated by setting $R_1 = 2.5$ instead of $R_1 = 1.7$. With $R_1 = 2.5$, it is still possible to obtain between three and four significant figure accuracy in the S-matrix elements obtained. If I were to rerun all the test problems, this is the integration parameter I would most carefully optimize.

In the analytic R-matrix propagation portion of each problem, two parameters governed the selection of step size. One parameter is BSTEP, which chooses step sizes according to the rate of change of the tract of the coupling matrix,[2] and the other is CUPMAX, which limits step sizes by the rate of change of the locally adiabatic basis.[2] Only in the second test problem was CUPMAX set to a value which affected any of the step sizes. The effect can be seen in Table IIB in that more time was expended from $6a_o$ to $7a_o$ than on either side of this region. The step size algorithm used a very small value of STPMIN and a large value of STPMAX.

My experience with the step size algorithm based on BSTEP[2] has been that it tends to take too small a step in the hard wall region of the potential, when BSTEP is set so that proper step sizes are used in the long-range region of the potential. Once again, if I were to rerun the test problems, I would more carefully optimize (increase) the STPMIN parameter.

In conclusion, the test problems selected by the director of the NRCC workshop on close coupling methods have fulfilled the criterion of presenting potentials which would be encountered in realistic research problems. The L^2/analytic hybrid method used here is not the optimal choice for these problems. The L^2 method needs further work to reduce, if possible, the effort expended at the first scattering energy. The program used is limited to fairly small systems of coupled equations because of computer core restrictions. The L^2 method seems also to get comparatively worse as the number of coupled channels increases.

Table I. Integration Regions for the Hybrid R-matrix Method

Problem	J_{TOTAL}	N_{CHAN}	N_D	N_{BOX}	N_{PROP}	$R_1(a_o)$	$R_2(a_o)$	$R_e(a_o)$	T_1(sec)	R_w(sec)
1	4	2	12	33	252	1.7	11.60	35	0.53	0.13
1	4	8	48	15	356	1.7	6.20	35	6.96	1.08
1	4	18	108	5	182	1.7	3.20	35	22.52	3.69
2(3)	5	3	18	5	950(170)	3.3	4.80	700(7)	1.51(0.40)	0.18(0.02)
2(3)	5	6	36	5	1029(168)	3.3	4.80	700(7)	4.51(1.41)	2.37(0.37)
2(3)	5	15	75	6	1296(271)	3.3	4.20	700(7)	41.42(14.04)	21.85(5.88)
2(3)	25	3	18	10	284(12)	3.3	6.30	700(7)	0.67(0.32)	0.58(0.12)
2(3)	25	10	60	7	544(53)	3.3	5.05	700(7)	9.67(4.70)	1.59(0.30)
2(3)	25	22	110	3	733(183)	3.3	3.90	700(7)	63.33(23.55)	14.14(3.15)
4	5	4	24	8	208	5.0(-6)	2.40	50	0.82	0.19
4	5	15	60	6	85	5.0(-6)	1.80	50	6.60	1.23
4	5	19	76	4	96	5.0(-6)	1.20	50	13.33	3.03

Table IIA. Details of Timing for Test Problem 1*

Interval(a_o) R_{left}	R_{right}	Method	N_{STEPS}	Total Time (sec)	Time/a_o (sec)
1.7	3.2	L^2	5	14.77(0.47)	9.85(0.31)
3.2	4.0	analytic	47	1.98(0.80)	2.48(1.00)
4.0	5.0	analytic	32	1.35(0.55)	1.35(0.55)
5.0	6.0	analytic	17	0.72(0.29)	0.72(0.29)
6.0	8.0	analytic	14	0.59(0.24)	0.30(0.12)
8.0	10.0	analytic	10	0.42(0.17)	0.21(0.09)
10.0	14.0	analytic	16	0.67(0.27)	0.17(0.07)
14.0	20.0	analytic	18	0.76(0.31)	0.13(0.05)
20.0	35.0	analytic	28	1.19(0.48)	0.08(0.03)

*Total L^2 time was 14.77(0.47) sec; total analytic time was 7.67(3.11) sec; 18 channels.

Table IIB. Details of Timing for Test Problem 2a*

Interval(a_o) R_{left}	R_{right}	Method	N_{STEPS}	Total Time	Time/a_o
3.3	4.2	L^2	6	6.71(0.25)	7.45(0.28)
4.2	5.0	analytic	73	1.95(0.78)	2.44(0.98)
5.0	6.3	analytic	127	3.39(1.36)	2.63(1.05)
6.3	7.3	analytic	100	2.67(1.07)	2.67(1.07)
7.3	8.4	analytic	100	2.67(1.07)	2.43(0.97)
8.4	9.8	analytic	100	2.67(1.07)	1.91(0.77)
9.8	11.7	analytic	100	2.67(1.07)	1.41(0.56)
11.7	14.3	analytic	100	2.67(1.07)	1.03(0.41)
14.3	18.2	analytic	100	2.67(1.07)	0.69(0.27)
18.2	25.2	analytic	100	2.67(1.07)	0.38(0.15)
25.2	51.6	analytic	100	2.67(1.07)	0.10(0.04)
51.6	142.8	analytic	100	2.67(1.07)	0.03(0.01)
142.8	700	analytic	196	5.23(2.10)	0.003(0.001)

*Total L^2 time was 6.71(0.25) sec; total analytic time was 34.60(13.87) sec; 15 channels.

Table IIC. Details of Timing for Test Problem 2b*

Interval(a_o) R_{left}	R_{right}	Method	N_{STEPS}	Total Time (sec)	Time/a_o (sec)
3.3	5.0	L^2	3	10.08(0.47)	16.80(0.79)
3.9	5.0	analytic	107	7.72(3.11)	7.02(2.82)
5.0	5.7	analytic	43	3.10(1.25)	4.43(1.78)
5.7	7.5	analytic	50	3.61(1.45)	2.01(0.81)
7.5	10.1	analytic	50	3.61(1.45)	1.39(0.56)
10.1	12.3	analytic	50	3.61(1.45)	1.64(0.66)
12.3	14.6	analytic	50	3.61(1.45)	1.57(0.63)
14.6	17.1	analytic	50	3.61(1.45)	1.44(0.58)
17.1	21.3	analytic	50	3.61(1.45)	0.86(0.35)
21.3	34.9	analytic	50	3.61(1.45)	0.27(0.11)
34.9	72.7	analytic	50	3.61(1.45)	0.10(0.04)
72.7	146.7	analytic	50	3.61(1.45)	0.05(0.02)
146.7	700	analytic	183	13.21(5.32)	0.02(0.01)

*Total L^2 time was 10.080(0.47) sec; total analytic time was 52.91(21.29) sec; 22 channels.

Table IID. Details of Timing for Test Problem 4*

Interval(a_o) R_{left}	R_{right}	Method	N_{STEP}	Total Time (sec)	Time/a_o
0	1.2	L^2	3	7.09(0.47)	5.91(0.39)
1.2	2.0	analytic	15	0.96(0.38)	1.12(0.48)
2.0	3.0	analytic	10	0.64(0.26)	0.64(0.26)
3.0	4.6	analytic	10	0.64(0.26)	0.41(0.16)
4.6	6.8	analytic	10	0.64(0.26)	0.29(0.12)
6.8	10.1	analytic	10	0.64(0.26)	0.19(0.078)
10.1	15.0	analytic	10	0.64(0.26)	0.13(0.052)
15.0	22.2	analytic	10	0.64(0.26)	0.088(0.035)
22.2	32.9	analytic	10	0.64(0.26)	0.060(0.024)
32.9	50.0	analytic	11	0.70(0.28)	0.041(0.016)

*Total L^2 time was 7.09(0.47) sec; total analytic time was 6.12(2.45) sec; 19 channels.

References

1. R. ~ Walker and B. I. Schneider, "An L^2 Approach to R-matrix propagation," NRCC close coupling workshop report, Vol. 1. See also, B. I. Schneider and R. B. Walker, J. Chem. Phys. 70, 2466 (1979).
2. E. B. Stechel, R. B. Walker, and J. C. Light, J. Chem. Phys. 69, 3518 (1978).